# wwPDB NMR Structure Validation Summary Report

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|---|---|---|
| PDB ID | : | 2M30 |
| BMRB ID | : | 7376 |
| Title | : | Solution NMR refinement of a metal ion bound protein using quantum mechanical/molecular mechanical and molecular dynamics methods |
| Authors | : | Chakravorty, D.K.; Wang, B.I.; Lee, C.I.; Guerra, A.J.; Giedroc, D.P.; Merz Jr., K.M.; Arunkumar, A.I.; Pennella, M.; Kong, X. |
| Deposited on | : | 2013-01-04 |

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

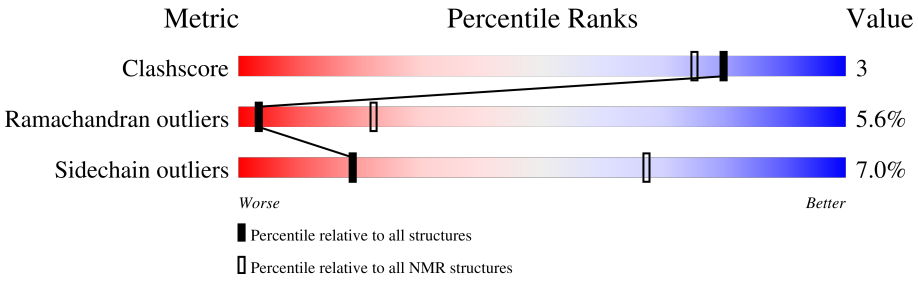
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| wwPDB-RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| wwPDB-ShiftChecker | : | v1.2 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36.2 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 26%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




| Metric | Whole archive (#Entries) | NMR archive (#Entries) |
|---|---|---|
| Clashscore | 158937 | 12864 |
| Ramachandran outliers | 154571 | 11451 |
| Sidechain outliers | 154315 | 11428 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 106 | 62% 17% • 7% 10% |
| 1 | B | 106 | 61% 16% • 8% 10% |

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

The following residues are included in the computation of the global validation metrics.

| Well-defined (core) protein residues | | | |
|---|---|---|---|
| **Well-defined core** | **Residue range (total)** | **Backbone RMSD (Å)** | **Medoid model** |
| 1 | A:10-A:73, A:78-A:101, B:10-B:72, B:78-B:100 (174) | 0.52 | 8 |

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 1 clusters. No single-model clusters were found.

| Cluster number | Models |
|---|---|
| 1 | 1, 2, 3, 4, 5, 6, 7, 8, 9, 10 |

# 3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3058 atoms, of which 1546 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Repressor protein.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 95 | Total | C | H | N | O | S | 0 |
| | | | 1528 | 471 | 773 | 141 | 140 | 3 | |
| 1 | B | 95 | Total | C | H | N | O | S | 0 |
| | | | 1528 | 471 | 773 | 141 | 140 | 3 | |

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | |
|---|---|---|---|---|
| 2 | A | 1 | Total | Zn |
| | | | 1 | 1 |
| 2 | B | 1 | Total | Zn |
| | | | 1 | 1 |

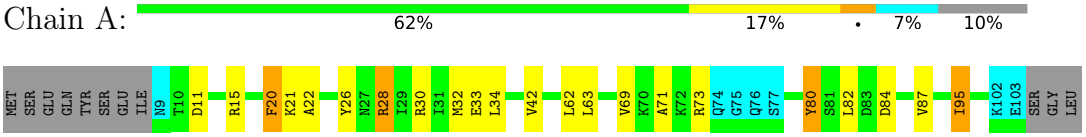
# 4 Residue-property plots

## 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

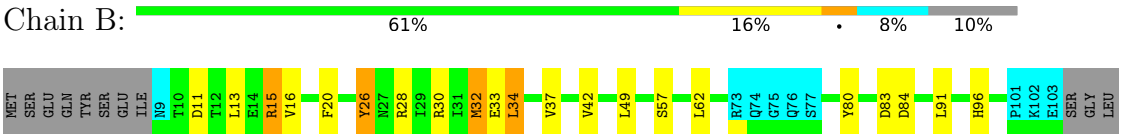
• Molecule 1: Repressor protein

Chain A:




• Molecule 1: Repressor protein

Chain B:

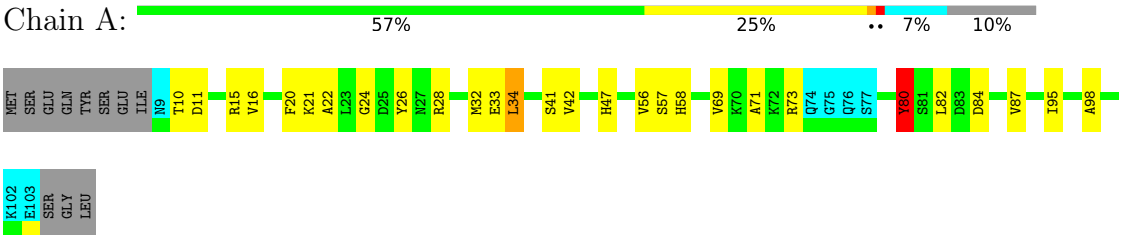



## 4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 8. Colouring as in section 4.1 above.

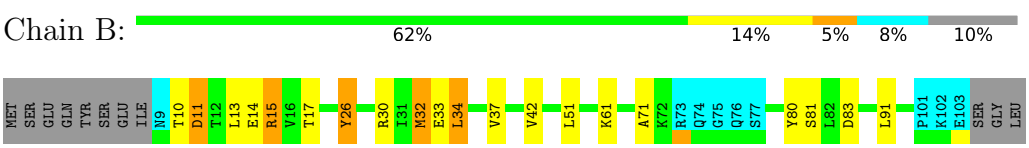
• Molecule 1: Repressor protein

Chain A:




• Molecule 1: Repressor protein

Chain B:



# 5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics and quantum mechanical molecular mechanical molecular dynamics*.

Of the 132000 calculated structures, 10 were deposited, based on the following criterion: *Structures from 1 ns of independent QM/MM MD sampling*.

The following table shows the software used for structure solution, optimisation and refinement.

| Software name | Classification | Version |
|---|---|---|
| Amber | structure solution | 11 |
| Amber | refinement | 11 |
| Amber | geometry optimization | 11 |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

| Chemical shift file(s) | working_cs.cif |
|---|---|
| Number of chemical shift lists | 1 |
| Total number of shifts | 730 |
| Number of shifts mapped to atoms | 671 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 59 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 26% |

# 6 Model quality (i)

## 6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #Z>5 | RMSZ | #Z>5 |
| 1 | A | 1.46±0.04 | 2±1/713 ( 0.3± 0.2%) | 1.97±0.08 | 18±4/963 ( 1.9± 0.4%) |
| 1 | B | 1.42±0.05 | 2±1/694 ( 0.2± 0.1%) | 1.88±0.10 | 15±3/938 ( 1.6± 0.4%) |
| All | All | 1.44 | 40/14070 ( 0.3%) | 1.93 | 335/19010 ( 1.8%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | Chirality | Planarity |
|---|---|---|---|
| 1 | A | 0.0±0.0 | 4.0±2.1 |
| 1 | B | 0.0±0.0 | 3.6±1.3 |
| All | All | 0 | 76 |

5 of 37 unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | A | 30 | ARG | CZ-NH1 | -9.20 | 1.21 | 1.33 | 3 | 1 |
| 1 | B | 46 | SER | CB-OG | -8.41 | 1.31 | 1.42 | 6 | 1 |
| 1 | A | 46 | SER | CB-OG | -8.02 | 1.31 | 1.42 | 7 | 1 |
| 1 | A | 38 | SER | CB-OG | 7.44 | 1.51 | 1.42 | 1 | 1 |
| 1 | A | 15 | ARG | CZ-NH1 | -7.28 | 1.23 | 1.33 | 5 | 1 |

5 of 168 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | A | 15 | ARG | NE-CZ-NH1 | 18.35 | 129.48 | 120.30 | 9 | 10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | B | 30 | ARG | NE-CZ-NH1 | 18.30 | 129.45 | 120.30 | 2 | 7 |
| 1 | A | 30 | ARG | NE-CZ-NH1 | 16.54 | 128.57 | 120.30 | 10 | 9 |
| 1 | B | 15 | ARG | NE-CZ-NH1 | 16.39 | 128.50 | 120.30 | 2 | 6 |
| 1 | B | 30 | ARG | NE-CZ-NH2 | -15.89 | 112.35 | 120.30 | 2 | 5 |

There are no chirality outliers.

5 of 30 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Group | Models (Total) |
|---|---|---|---|---|---|
| 1 | A | 32 | MET | Peptide | 9 |
| 1 | B | 32 | MET | Peptide | 9 |
| 1 | A | 80 | TYR | Sidechain | 7 |
| 1 | A | 20 | PHE | Peptide,Sidechain | 6 |
| 1 | A | 30 | ARG | Sidechain | 3 |

## 6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|---|---|---|---|---|---|
| 1 | A | 701 | 724 | 724 | 4±2 |
| 1 | B | 683 | 704 | 704 | 5±2 |
| All | All | 13860 | 14280 | 14280 | 76 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

5 of 47 unique clashes are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:45:ILE:HG23 | 1:B:49:LEU:HD13 | 0.68 | 1.66 | 4 | 2 |
| 1:A:71:ALA:HB2 | 1:A:80:TYR:CE2 | 0.67 | 2.25 | 8 | 5 |
| 1:B:34:LEU:C | 1:B:34:LEU:HD13 | 0.57 | 2.20 | 4 | 4 |
| 1:A:13:LEU:O | 1:A:17:THR:HG23 | 0.56 | 2.01 | 4 | 1 |
| 1:A:34:LEU:C | 1:A:34:LEU:HD13 | 0.55 | 2.21 | 8 | 2 |

## 6.3 Torsion angles (i)

### 6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 88/106 (83%) | 70±2 (80±3%) | 11±3 (13±3%) | 6±2 (7±2%) | 2 | 16 |
| 1 | B | 86/106 (81%) | 74±3 (86±3%) | 8±3 (10±3%) | 3±1 (4±1%) | 5 | 31 |
| All | All | 1740/2120 (82%) | 1443 (83%) | 199 (11%) | 98 (6%) | 3 | 22 |

5 of 19 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 42 | VAL | 10 |
| 1 | B | 42 | VAL | 10 |
| 1 | A | 22 | ALA | 9 |
| 1 | A | 28 | ARG | 8 |
| 1 | A | 33 | GLU | 7 |

### 6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 80/96 (83%) | 74±2 (93±3%) | 6±2 (7±3%) | 19 | 68 |
| 1 | B | 78/96 (81%) | 72±1 (93±1%) | 6±1 (7±1%) | 18 | 67 |
| All | All | 1580/1920 (82%) | 1470 (93%) | 110 (7%) | 19 | 67 |

5 of 43 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | B | 13 | LEU | 10 |
| 1 | A | 95 | ILE | 9 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 1 | A | 34 | LEU | 7 |
| 1 | B | 26 | TYR | 7 |
| 1 | A | 87 | VAL | 6 |

### 6.3.3 RNA

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.5 Carbohydrates

There are no monosaccharides in this entry.

## 6.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

## 6.7 Other polymers

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

# 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 26% for the well-defined parts and 25% for the entire structure.

## 7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

### 7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

| | |
|---|---|
| Total number of shifts | 730 |
| Number of shifts mapped to atoms | 671 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 59 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 0 |

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. First 5 (of 59) occurrences are reported below.

| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---|---|---|---|---|---|---|---|
| | | | | | Value | Uncertainty | Ambiguity |
| 1 | A | 2 | ALA | CA | 51.528 | 0.400 | 1 |
| 1 | A | 2 | ALA | CB | 18.91 | 0.400 | 1 |
| 1 | A | 3 | GLU | H | 8.66 | 0.020 | 1 |
| 1 | A | 3 | GLU | C | 176.132 | 0.400 | 1 |
| 1 | A | 3 | GLU | CA | 59.126 | 0.400 | 1 |
| 1 | A | 3 | GLU | CB | 28.842 | 0.400 | 1 |
| 1 | A | 3 | GLU | N | 120.962 | 0.400 | 1 |
| 1 | A | 4 | GLN | H | 8.442 | 0.020 | 1 |
| 1 | A | 4 | GLN | HE21 | 7.414 | 0.020 | 2 |
| 1 | A | 4 | GLN | HE22 | 6.798 | 0.020 | 2 |
| 1 | A | 4 | GLN | C | 175.591 | 0.400 | 1 |
| 1 | A | 4 | GLN | CA | 55.755 | 0.400 | 1 |
| 1 | A | 4 | GLN | CB | 29.475 | 0.400 | 1 |
| 1 | A | 4 | GLN | N | 122.004 | 0.400 | 1 |

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| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---|---|---|---|---|---|---|---|
| | | | | | Value | Uncertainty | Ambiguity |
| 1 | A | 4 | GLN | NE2 | 111.932 | 0.400 | 1 |
| 1 | A | 5 | TYR | H | 8.305 | 0.020 | 1 |
| 1 | A | 5 | TYR | CA | 57.668 | 0.400 | 1 |
| 1 | A | 5 | TYR | CB | 38.067 | 0.400 | 1 |
| 1 | A | 5 | TYR | N | 121.338 | 0.400 | 1 |
| 1 | A | 6 | SER | H | 7.988 | 0.020 | 1 |
| 1 | A | 6 | SER | C | 173.873 | 0.400 | 1 |
| 1 | A | 6 | SER | CA | 57.59 | 0.400 | 1 |
| 1 | A | 6 | SER | CB | 63.618 | 0.400 | 1 |
| 1 | A | 6 | SER | N | 118.236 | 0.400 | 1 |
| 1 | A | 7 | GLU | H | 8.286 | 0.020 | 1 |
| 1 | A | 7 | GLU | C | 175.802 | 0.400 | 1 |
| 1 | A | 7 | GLU | CA | 56.31 | 0.400 | 1 |
| 1 | A | 7 | GLU | CB | 29.88 | 0.400 | 1 |
| 1 | A | 7 | GLU | N | 123.02 | 0.400 | 1 |
| 1 | A | 8 | ILE | H | 8.101 | 0.020 | 1 |
| 1 | A | 8 | ILE | HD11 | 0.772 | 0.020 | 1 |
| 1 | A | 8 | ILE | HD12 | 0.772 | 0.020 | 1 |
| 1 | A | 8 | ILE | HD13 | 0.772 | 0.020 | 1 |
| 1 | A | 8 | ILE | C | 175.128 | 0.400 | 1 |
| 1 | A | 8 | ILE | CA | 60.246 | 0.400 | 1 |
| 1 | A | 8 | ILE | CB | 37.568 | 0.400 | 1 |
| 1 | A | 8 | ILE | CD1 | 12.321 | 0.400 | 1 |
| 1 | A | 8 | ILE | N | 121.13 | 0.400 | 1 |
| 1 | A | 104 | SER | H | 8.367 | 0.020 | 1 |
| 1 | A | 104 | SER | C | 174.942 | 0.400 | 1 |
| 1 | A | 104 | SER | CA | 58.258 | 0.400 | 1 |
| 1 | A | 104 | SER | CB | 63.548 | 0.400 | 1 |
| 1 | A | 104 | SER | N | 116.875 | 0.400 | 1 |
| 1 | A | 105 | GLY | H | 8.381 | 0.020 | 1 |
| 1 | A | 105 | GLY | C | 173.181 | 0.400 | 1 |
| 1 | A | 105 | GLY | CA | 45.047 | 0.400 | 1 |
| 1 | A | 105 | GLY | N | 111.32 | 0.400 | 1 |
| 1 | A | 106 | LEU | H | 7.723 | 0.020 | 1 |
| 1 | A | 106 | LEU | HD11 | 0.838 | 0.020 | 2 |
| 1 | A | 106 | LEU | HD12 | 0.838 | 0.020 | 2 |
| 1 | A | 106 | LEU | HD13 | 0.838 | 0.020 | 2 |
| 1 | A | 106 | LEU | HD21 | 0.875 | 0.020 | 2 |
| 1 | A | 106 | LEU | HD22 | 0.875 | 0.020 | 2 |
| 1 | A | 106 | LEU | HD23 | 0.875 | 0.020 | 2 |
| 1 | A | 106 | LEU | CA | 56.233 | 0.400 | 1 |

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| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---|---|---|---|---|---|---|---|
| | | | | | Value | Uncertainty | Ambiguity |
| 1 | A | 106 | LEU | CB | 43.101 | 0.400 | 1 |
| 1 | A | 106 | LEU | CD1 | 23.405 | 0.400 | 1 |
| 1 | A | 106 | LEU | CD2 | 25.12 | 0.400 | 1 |
| 1 | A | 106 | LEU | N | 127.393 | 0.400 | 1 |

### 7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction ± precision, *ppm* | Suggested action |
|---|---|---|---|
| $^{13}C_{\alpha}$ | 105 | -0.38 ± 0.24 | None needed (< 0.5 ppm) |
| $^{13}C_{\beta}$ | 96 | 0.49 ± 0.28 | None needed (< 0.5 ppm) |
| $^{13}C'$ | 100 | -0.59 ± 0.19 | Should be applied |
| $^{15}N$ | 103 | 0.59 ± 0.43 | None needed (imprecise) |

### 7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 26%, i.e. 631 atoms were assigned a chemical shift out of a possible 2465. 0 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | $^{1}H$ | $^{13}C$ | $^{15}N$ |
|---|---|---|---|---|
| Backbone | 348/872 (40%) | 87/351 (25%) | 174/348 (50%) | 87/173 (50%) |
| Sidechain | 283/1425 (20%) | 150/937 (16%) | 127/439 (29%) | 6/49 (12%) |
| Aromatic | 0/168 (0%) | 0/90 (0%) | 0/62 (0%) | 0/16 (0%) |
| Overall | 631/2465 (26%) | 237/1378 (17%) | 301/849 (35%) | 93/238 (39%) |

### 7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

### 7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble

composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A: